

Methyl pivalate
598-98-1 | DTXSID4027234

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 23.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 8.22e-01

Nearest Neighbors from the Training Set

Image not found

3-Methylaniline

Measured: 33.9

Predicted: 33.3

Image not found

Benzamide

Measured: 28.8

Predicted: 29.7

Image not found

Benzoic acid

Measured: 31.6

Predicted: 35.5

Image not found

4-Vinylpyridine

Measured: 15.1

Predicted: 43.8

Image not found

Benzyl alcohol

Measured: 12.6

Predicted: 20.1